CRCS, Inc

WORKING DRAFT

INFORMATION REVIEW

Perfluorooctanesulfonyl fluoride

IR 356
SEPTEMBER 22, 1983

PREPARED UNDER EPA CONTRACT No. 68-01-6650 FOR:
TSCA INTERAGENCY TESTING COMMITTEE

SUBMITTED BY:

CRCS, INC
11701 BOWMAN GREEN DR
RESTON, VA 22090

N O T I C E

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PREFACE

This report was prepared by a multidisciplinary team of scientists and technicians. Dr. Satish Bhalla was the principal author and compiler.

The information resources used in preparing this review include automated data bases, journal articles, general reference materials, contractor/ agency reports, and unpublished data provided by industry.

The authors wish to acknowledge the contributions of data by:

W. H. Pearlson of the 3M Company
A. Fankhanel of Mercantile Development Inc.

Perfluorooctanesulfonyl Fluoride

OVERVIEW

CHARACTERISTICS

Perfluorooctanesulfonyl fluoride (POSF) is a clear, low viscosity liquid with an estimated log octanol/water partition coefficient of 1.4.

PRODUCTION AND USE

The TSCA Inventory lists an annual production in 1977 of 1 to 10 million pounds for this compound. Current annual production is in excess of 1 million pounds. POSF is a chemical intermediate used in the manufacture of fabric treatment and surfactant fluorochemicals. Occupational exposure to POSF is low.

BIOCHEMICAL INFORMATION

No information was found.

TOXICOLOGICAL INFORMATION

Mutagenicity assays were negative. The intravenous LD_{50} of POSF in the mouse was in excess of 300 mg/kg.

ENVIRONMENTAL INFORMATION

At most, 2500 pounds of POSF may be released into the atmosphere each year. It is expected to partition to water, soil, and sediment where it will slowly hydrolyze and biodegrade.

SUMMARY OF HAZARD POTENTIAL

Little information is available on health and environmental effects of the compound. Occupational and environmental exposure appear to be low.

Perfluorooctanesulfonyl Fluoride

I. CHEMICAL AND PHYSICAL INFORMATION

A. IDENTIFICATION

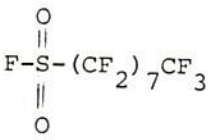
CAS No.: 307-35-7

NIOSH No.: Not available

Synonyms: POSF
1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro- (9CI)

B. FORMULAS AND MOLECULAR WEIGHT

Structural Formula:



Empirical Formula: $C_8F_{18}O_2S$

Molecular Weight: 502

C. PHYSICAL PROPERTIES (3M, 1982, unless otherwise noted)

Description: Clear low-viscosity liquid

Melting Point: No information found

Boiling Point: 154-155° C

Vapor Pressure: No information found

Specific Gravity: 1.8

Solubility in Water: A few ppm

Solubility in Organic Solvents: Soluble in diethyl ether and fluorinated solvents; slightly soluble in acetone, methanol and hydrocarbons.

Log Octanol/Water Partition Coefficient: 1.4 (estimated by the method of Hansch and Leo from Lyman et al., 1982)

D. CHEMICAL PROPERTIES

3M (1982) states that primarily because of low solubility, POSF is relatively unreactive in neutral and acidic aqueous media and can be steam distilled without significant hydrolysis. It reacts controllably with aqueous organic or inorganic strong bases at 50°C or slightly above to form the salt of the corresponding acid. In general, the salts have low solubility in water. In solution, POSF reacts vigorously and strongly exothermically with primary and secondary amines, and readily with any protic nucleophile in the presence of soluble base, even at room temperature.

E. EXPOSURE ESTIMATES

1. Production

The public portion of the TSCA Chemical Substances Inventory (TSCA Inventory, 1982) lists the 3M Company, Decatur, AL as a manufacturer of POSF, with production of 1 to 10 million pounds of the compound in 1977. Mercantile Development Inc., Westport, CT is also listed as an importer/small manufacturer who chose not to report production for 1977 (see Enclosure 1). Mercantile Development (1983) does not currently produce or import POSF. 3M (1982) confirmed sole domestic production of the compound at a current annual rate in excess of 1 million pounds.

POSF can be prepared via batch electrolysis of a 10% (wt.) solution of n-octanesulfonyl chloride in anhydrous liquid hydrogen fluoride at 1 atmosphere and 17-19°C. An insoluble liquid phase is formed during electrolysis which settles to the bottom of the cell. Withdrawal and distillation of this layer gives POSF in 30-35% molar yields. Hydrolysis of the sulfonyl fluoride with potassium hydroxide forms the potassium salt of POSF (Kirk-Othmer, 1979).

2. Use

3M (1983) reported that POSF is a chemical intermediate used in the manufacture of 3M's fabric treatment and surfactant fluorochemical lines.

Perfluorinated organic compounds are important industrial surfactants, textile treatment agents, surfactant intermediates, and oil- and water-repellent lubricants (Kirk-Othmer, 1979; Comninellis et al., 1975). Salts of octane and longer chain perfluoroalkane sulfonic acids are surface-active agents in aqueous media. The unique surface-active properties (e.g. chemical and thermal stability, low surface tensions) of the salts of these acids have led to the use of a number of commercial fluorochemical surfactants as wetting and leveling agents (Kirk-Othmer, 1980).

3. Occupational Exposure

POSF is manufactured, stored and processed in closed systems. Approximately 100 workers are potentially exposed to less than 0.5 ppm POSF in plant air on a regular basis. An additional 30 workers, in other 3M manufacturing units to which about 100 55-gallon drums of the compound are shipped, are also exposed to the same ambient air concentrations for less than 5 days per year (3M, 1982).

4. Releases

Atmospheric releases of POSF occur at manholes and drum filling stations. Tar-like manufacturing byproducts, containing no more than 1 or 2% POSF, are landfilled or sent to the plant's biological wastewater treatment facility. Losses during purification (principally fumes collected in water scrubbers) and occasional spills are also routed to the wastewater treatment plant. No more than 3000, 7500, and 2500 pounds of POSF are estimated to be released annually to landfills, wastewater treatment facility and the atmosphere, respectively (3M, 1982).

F. SCORES FROM 4th ITC EXERCISE

1. Occupational and Consumer Exposure

The exposure scores for perfluorooctanesulfonyl fluoride (normalized from 0.0 to 1.0) are as follows:

Occupational Exposure Index	0.44
Near Plant Exposure Index	0.17
Environmental Exposure Index	0.22
General Population Exposure Index	0.13

2. Health and Environmental Effects

Health and environmental effects were scored on a scale from 0 to 3 (minus assigned if score is based solely on judgment in the absence of experimental data).

Individual factor scores for perfluorooctanesulfonyl fluoride:

Mutagenicity	-1.0
Carcinogenicity	-1.0
Teratogenicity	-1.5
Reproductive effects	-1.0
Acute toxicity effects	-2.0
Other toxic effects	-2.0
Bioaccumulation	-2.0
Ecological effects	-2.0

II. BIOCHEMICAL INFORMATION

A. METABOLISM

No information found

B. EFFECTS ON ENZYMES AND OTHER BIOCHEMICAL ASPECTS

No information found

III. TOXICOLOGICAL INFORMATION

A. CARCINOGENICITY

No information found

B. GENTOXICITY

Mutagenicity tests--the Ames Salmonella typhimurium bacteria strains TA1535, TA1537, TA1538, TA98, and TA100 and the yeast recombinant assay using Saccharomyces cerevisiae D3 strain--were negative. Each strain was tested with and without metabolic activiation (3M, 1982).

C. TERATOGENICITY, EMBRYOTOXICITY, AND FETOTOXICITY

No information found

D. SPECIAL STUDIES

Sulfonyl fluorides, which may contain small amount of hydrogen fluoride, are irritating to skin, eye, and respiratory system (3M, 1982).

E. ACUTE TOXICITY

When POSF was applied to the skin of mice at the level of 200 mg/kg body weight, no indications of toxicity were observed. The intravenous LD_{50} in mouse of POSF was in excess of 300 gm/kg (3M, 1982).

F. SHORT-TERM STUDIES (SUB-CHRONIC)

No information found

G. LONG-TERM STUDIES (CHRONIC)

No information found

IV. OBSERVATIONS IN HUMANS

No information found

V. ENVIRONMENTAL INFORMATION

A. ENVIRONMENTAL RELEASE AND CONCENTRATIONS

1. Environmental Entry

3M (1982) reports that a maximum of 7500 pounds per year of POSF is disposed of in their on-site biological wastewater treatment facility. These liquids are from reaction waste streams, water scrubbers, and inadvertent spills. No more than 3000 pounds per year of POSF in tar-like byproducts are landfilled. Release into the atmosphere is at most 2500 pounds per year.

2. Environmental Concentrations

No information found

B. ENVIRONMENTAL FATE

Very little information was found on the environmental fate of POSF. In the following comments we project the environmental fate of the compound based on the available data and physical and chemical properties.

1. Partitioning Among Environmental Compartments

The low affinity of POSF for solubilizing in water, its slight solubility in hydrocarbons, its moderate edtimated octanol/water partition coefficient, and its high molecular weight indicate it will prefer the soil and sediment slightly over water but the large volume of water present in the environment will result in a significant portion of POSF residing in the water.

2. Aquatic Chemistry

POSF released to the environment can be expected to hydrolyze slowly to a water soluble sulfonic acid salt, more rapidly in strongly basic soils (3M, 1982).

3. Atmospheric Chemistry

Due to its high boiling point and high molecular weight POSF is not expected to reside in the atmosphere long enough for atmospheric chemistry to play a significant role in the environmental fate of the compound.

4. Biodegradation

The fluorine in POSF will inhibit biodegradation. Therefore, biodegradation of POSF should occur slowly in the environment.

5. Bioconcentration

The low estimated log octanol/water partition coefficient and its slight solubility in organics indicate POSF will not bioconcentrate to any appreciable extent.

6. Summary

POSF is expected to partition to water, soil, and sediment where it will slowly hydrolyze and biodegrade.

C. ECOLOGICAL EFFECTS

No information found

Comment

3M (1982) provided the following aquatic toxicity data for FLUORAD FC-95 (100% potassium perfluoroalkylsulfonates):

Species	96-hr LC_{50} (95% confidence interval)
Fathead minnow (*Pimephales promelas*)	38 mg/l (28-50 mg/l)
Bluegill sunfish (*Lepomis macrochirus*)	68 mg/l (62-74 mg/l)
Rainbow trout (*Salmo gairdneri*)	11 mg/l (9-13 mg/l)
	48-hr LC_{50} (95% confidence interval)
Water flea (*Daphnia magna*)	50 mg/l (43-56 mg/l)

In a 30 day critical lifestage test with fathead minnow egg-fry, a no effect level of 0.2 mg/l was found. Radiolabeled FC-95 at 1.9 mg/l caused statistically significant ($P_{0.05}$) reduction in survival of the fry but did not significantly ($P_{0.05}$) affect hatchability, weight, and length of the test organisms.

Microbial Toxicity:

Glucose metabolism (as oxygen uptake rate) by an activated sludge microbial population was not inhibited by FC-95 at concentrations of up to 4000 mg/l in Warburg respirometric studies (3M, 1982).

VI. DATA BASES SEARCHED

MEDLARS

Data Base	Time Coverage
MEDLINE	1966-present
CHEMLINE	
RTECS	
TDB (Toxicology Data Bank)	1977-present
TOXLINE	1979-present
TOX 74	1974-1978
TOX 65	1965-1973
CANCERLIT	1967-present
CANCERPROJ	1967-present

DIALOG

Data Base	Time Coverage
AGRICOLA	1970-present
APTIC	1966-1978
AQUACULTURE	1970-present
AQUALINE	1974-present
AQUATIC SCIENCES & FISHERIES ABSTRACTS	1978-present
BIOSIS PREVIEWS	1969-present
CAB ABSTRACTS	1973-present
CA SEARCH	1967-present
CDI (Comprehensive Dissert. Index)	1961-present
CIN (Chem. Indust. Notes)	1974-present
CLAIMS/US PATENT ABSTRACTS	1971-present
COMPENDEX	1970-present
CONFERENCE PAPERS INDEX	1973-present
CRGS (Chemical Regs. & Guidelines Systems)	1981-present
CRIS/USDA	1974-present
ENVIROLINE	1971-present
ENVIRONMENTAL BIBLIOGRAPHY	1974-present
EXCERPTA MEDICA	1974-present
FOODS ADLIBRA	1974-present
FSTA (Food Science & Technology Abstracts)	1969-present
INSPEC	1969-present
INTERNATIONAL PHARM. ABS	1970-present
IRL (Life Sciences Collection)	1978-present
ISMEC	1973-present
NTIS	1970-present
OCEANIC ABSTRACTS	1964-present
PAPERCHEM	1968-present
PHARM. NEWS INDEX	1975-present
PTS PROMT	1972-present
PTS PREDALERT	1972-present

Perfluorooctanesulfonyl Fluoride

Data Base	Time Coverage
SCISEARCH	1974-present
SOCIAL SCISEARCH	1972-present
SSIE (Current Research)	1979-present
SURFACE COATING ABSTRACTS	1976-present
WELDASEARCH	1967-present
WORLD TEXTILES	1970-present

OTHER

Data Base	Time Coverage
APILIT	1964-present
APIPAT	1964-present
CIS/SANSS/OHMTADS	
EMIC	1940-present
P/E NEWS	1975-present
PESTDOC	1968-present
RINGDOC	1964-present
SAFETY	1975-present
STORET	
TITUS	1967-present
TSCA Inventory	
WPI	1963-present
WRA	

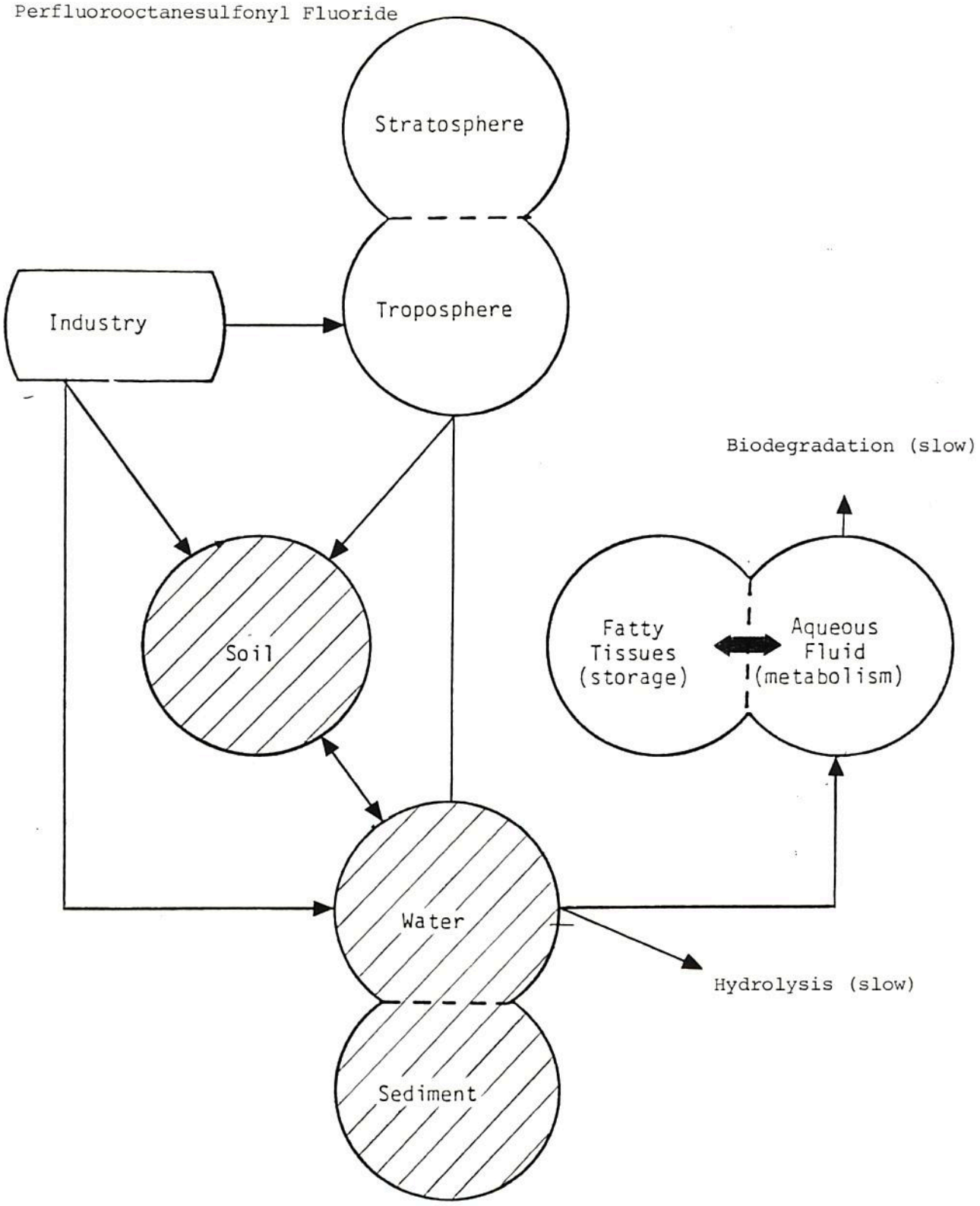


Figure 1. Projected environmental fate of POSF. Cross hatching indicates compartments in which the compound will tend to partition and slowly degrade.

307-35-7 1-Octanesulfonyl fluoride, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8=-heptadecafluoro-

3M COMPANY (005003R)
P.O. BOX 2206 HWY 20
WEST OF DECATUR
DECATUR AL 35602
MANUFACTURER
1977 PRODUCTION OF 1 MILLION TO TEN MILLION POUNDS

MERCANTILE DEVELOPMENT INC. (005408B)
274 RIVERSIDE AVE
WESTPORT CT 06880
IMPORTER
SMALL MANUFACTURER

CITED REFERENCES

Comninellis C., Philippe J. Plattner E. 1975. Process for the electrochemical fluorination of organic acid halides; hydrogen fluoride electrolyte. U.S. Patent No. 3919057.

Kirk-Othmer. 1979. Kirk-Othmer Encyclopedia of Chemical Technology. Vol. 10, 3rd ed., New York, NY: John Wiley & Sons. pg. 954.

Lyman W. J., Reehl W. F., Roseblatt D. H. 1982. Handbook of Chemical Property Estimation Methods. McGraw-Hill Book Company. New York, NY. Chapters 1, 2.

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